

STN-Structure Search

8/16/08

10/520,421

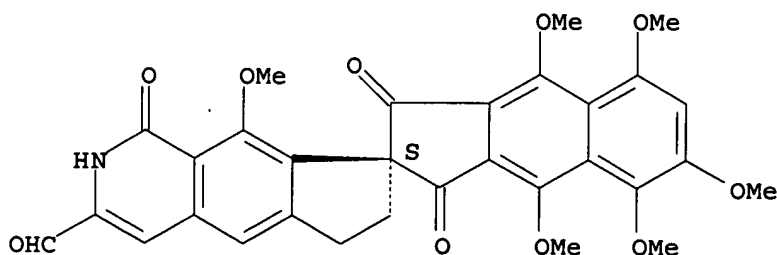
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L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:187890 CAPLUS
 DOCUMENT NUMBER: 134:353198
 TITLE: Enantioselective Total Synthesis of a Potent Antitumor Antibiotic, Fredericamycin A
 AUTHOR(S): Kita, Yasuyuki; Higuchi, Kazuhiro; Yoshida, Yutaka; Iio, Kiyosei; Kitagaki, Shinji; Ueda, Koichiro; Akai, Shuji; Fujioka, Hiromichi
 CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Osaka University, Suita Osaka, 565-0871, Japan
 SOURCE: Journal of the American Chemical Society (2001), 123(14), 3214-3222
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:353198

AB The asym. total synthesis of both enantiomers of the potent antitumor antibiotic fredericamycin A (I) is detailed based on the protocol for the construction of its peri-hydroxy polyarom. skeleton bearing the chirality at the spiro carbon via a strong base-induced cycloaddn. of suitably substituted homophthalic anhydrides (AB-ring unit) with an optically active CDEF-ring unit. Particular attention has been given to the novel synthesis of the optically active spiro carbon center by a stereospecific rearrangement of optically active benzofused-trans-epoxy acylates leading to spirocyclopentane-1,1'-indane systems. This method is quite useful for the construction of an optically active spiro compound and was applied to the synthesis of the optically pure CDEF-ring unit of I. Cycloaddn. of the optically pure CDEF-ring unit to AB-ring units prepared via benzyne afforded two natural and unnatural-type hexacyclic compds., which were converted to natural and unnatural enantiomers of synthetic I, and the absolute configuration of natural I was determined as S.

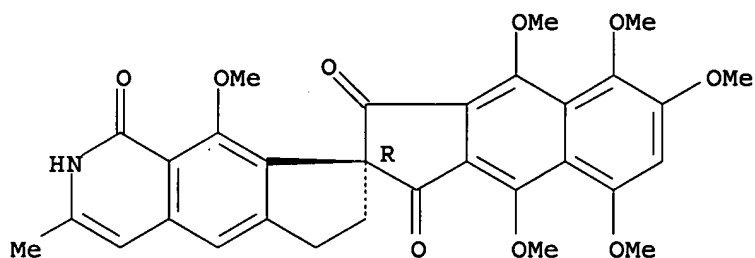
IT 225090-40-4P 225090-41-5P 259752-89-1P
 339151-76-7P 339151-77-8P 339151-78-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (enantioselective total synthesis of a potent antitumor antibiotic, fredericamycin A)
 RN 225090-40-4 CAPLUS
 CN Spiro[2H-benz[f]indene-2,8' - [8H]cyclopent[g]isoquinoline]-3'-carboxaldehyde, 1,1',2',3,6',7'-hexahydro-4,5,6,8,9,9'-hexamethoxy-1,1',3-trioxo-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 225090-41-5 CAPLUS
 CN Spiro[2H-benz[f]indene-2,8' - [8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 6',7'-tetrahydro-4,5,6,8,9,9'-hexamethoxy-3'-(1E,3E)-1,3-pentadienyl-, (2S)- (9CI) (CA INDEX NAME)

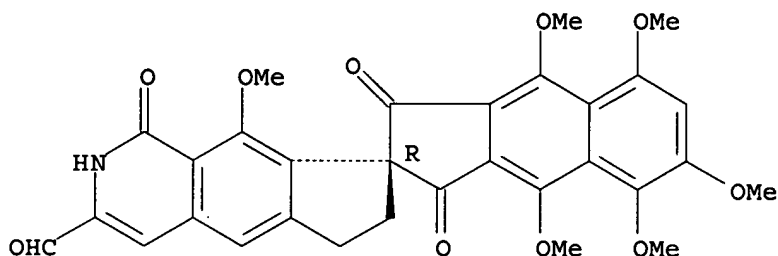
10/520,421



RN 339151-78-9 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-3'-carboxaldehyde, 1,1',2',3,6',7'-hexahydro-4,5,6,8,9,9'-hexamethoxy-1,1',3-trioxo-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 114 THERE ARE 114 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:151480 CAPLUS

DOCUMENT NUMBER: 132:194246

TITLE: Preparation of intermediates for novel antitumor spiro compounds, fredericamycin A and its analogs

INVENTOR(S): Kita, Yasuyuki; Fujioka, Hiromichi; Akai, Shuji; Higuchi, Kazuhiro

PATENT ASSIGNEE(S): Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000072752	A2	20000307	JP 1998-246347	19980831
PRIORITY APPLN. INFO.:			JP 1998-246347	19980831
OTHER SOURCE(S):			CASREACT 132:194246; MARPAT 132:194246	
GI				

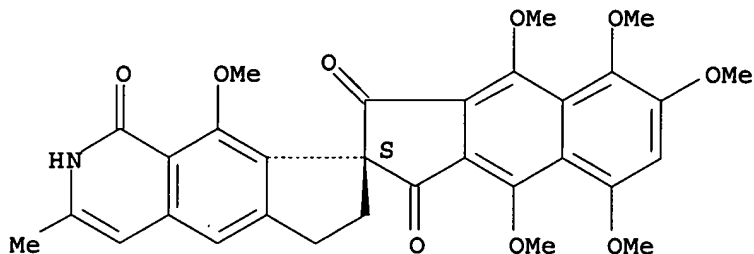
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The spiro compds. I [R1 = halo, alkyl which may be substituted with OH, alkoxy, or carboxy, CF3, CHO, Ac, alkylsulfonyl, alkanoyl, CO2H, CONH2,

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CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 6',7'-dihydro-4,5,6,8,9,9'-hexamethoxy-3'-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:192834 CAPLUS

DOCUMENT NUMBER: 130:352110

TITLE: Asymmetric total synthesis of fredericamycin A

AUTHOR(S): Kita, Yasuyuki; Higuchi, Kazuhiro; Yoshida, Yutaka; Iio, Kiyosei; Kitagaki, Shinji; Akai, Shuji; Fujioka, Hiromichi

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Osaka University, Suita, 565-0871, Japan

SOURCE: Angewandte Chemie, International Edition (1999), 38(5), 683-686

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The asym. total synthesis of fredericamycin A was accomplished via stereospecific rearrangement of the epoxy acylate and the regiocontrolled intermol. [4+2] cycloaddn. of homophthalic anhydrides to dienophiles and the absolute configuration of the single chiral center was established as (S).

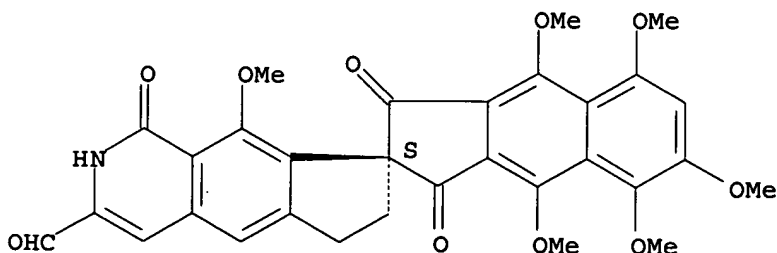
IT 225090-40-4P 225090-41-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (asym. synthesis of fredericamycin A)

RN 225090-40-4 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-3'-carboxaldehyde, 1,1',2',3,6',7'-hexahydro-4,5,6,8,9,9'-hexamethoxy-1,1',3-trioxo-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

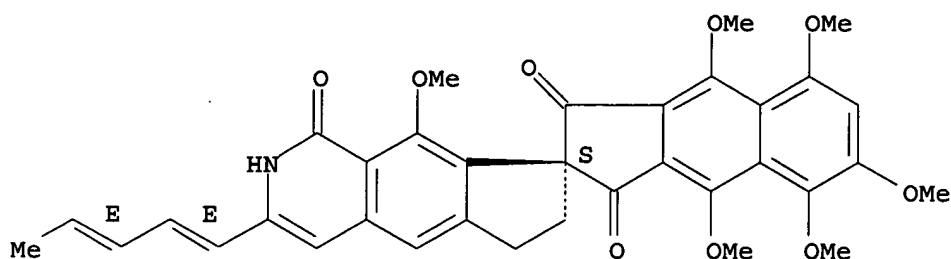


RN 225090-41-5 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 6',7'-tetrahydro-4,5,6,8,9,9'-hexamethoxy-3'-(1E,3E)-1,3-pentadienyl-, (2S)- (9CI) (CA INDEX NAME)

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Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:257730 CAPLUS

DOCUMENT NUMBER: 125:10466

TITLE: Further model studies related to fredericamycin A:
analogues in which ring C is expanded to six atoms, and
an examination of the diastereoselectivity of radical
spirocyclization

AUTHOR(S): Clive, Derrick L. J.; Kong, Xianglong; Paul, Christine
Chua

CORPORATE SOURCE: Chem. Dep., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.
SOURCE: Tetrahedron (1996), 52(17), 6085-116

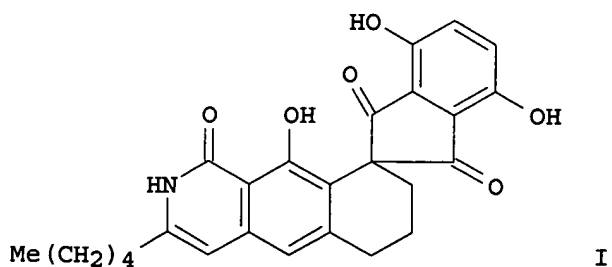
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PUBLISHER: Elsevier

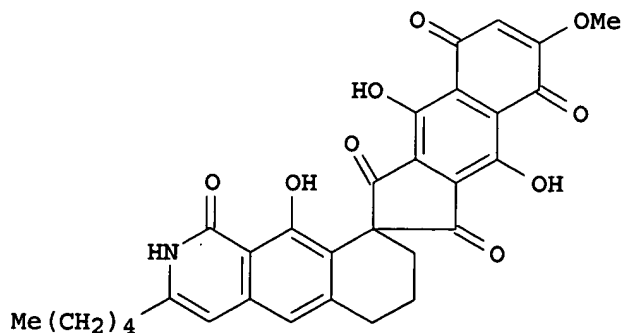
DOCUMENT TYPE: Journal

LANGUAGE: English

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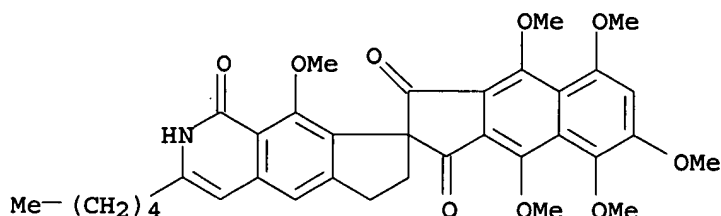
II

AB The fredericamycin A analogs I and II were synthesized. A key step is the process of radical spirocyclization, and the diastereoselectivity of this reaction was studied with model compds. In vitro tests showed that II was active against certain cell lines of colon and prostate cancer, while I was essentially inactive.

IT 176981-39-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (diastereoselectivity of radical spirocyclization in relation to preparation of fredericamycin A analogs)

RN 176981-39-8 CAPLUS

CN Spiro[2H-benz[f]indene-2,8']-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 6',7'-dihydro-4,5,6,8,9,9'-hexamethoxy-3'-pentyl- (9CI) (CA INDEX NAME)



L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:196595 CAPLUS

DOCUMENT NUMBER: 122:160324

TITLE: Total Synthesis of Crystalline (±)-Fredericamycin
 A. Use of Radical Spirocyclization

AUTHOR(S): Clive, Derrick L. J.; Tao, Yong; Khodabocus, Ahmad;
 Wu, Yong-Jin; Angoh, A. Gaetan; Bennett, Sharon M.;
 Boddy, Christopher N.; Bordeleau, Luc; Kellner, Dorit;
 et al.

CORPORATE SOURCE: Department of Chemistry, University of Alberta,
 Edmonton, AB, T6G 2G2, Can.

SOURCE: Journal of the American Chemical Society (1994),
 116(25), 11275-86
 CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:160324

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Crystalline (±)-fredericamycin A (I) was synthesized using, as a key step, 5-exo-digonal radical closure of selenide II. The selenide was generated from the corresponding ketone, itself assembled from two components: aldehyde III and bromonaphthalene IV. The product of the radical cyclization was converted into a spiro diketone, and the pentadienyl chain was then formed by a Wittig reaction. Selective deprotection of ring A was accompanied by isomerization of the diene system to the required E,E geometry, and treatment with boron tribromide, followed by aqueous hydrolysis in the presence of air, effected selective demethylation and oxidation to (±)-I. The radical spirocyclization used in this synthesis is a

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general method.

IT 145223-00-3P

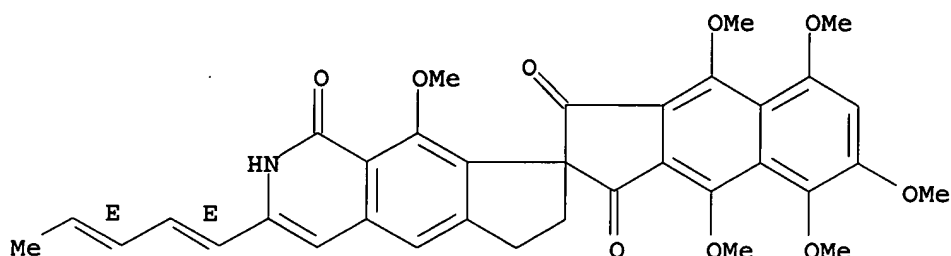
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(total synthesis of racemic fredericamycin A via radical spirocyclization)

RN 145223-00-3 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 6',7'-dihydro-4,5,6,8,9,9'-hexamethoxy-3'-(1E,3E)-1,3-pentadienyl-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:38651 CAPLUS

DOCUMENT NUMBER: 118:38651

TITLE: Total synthesis of (+)-fredericamycin A. Use of radical spirocyclization

AUTHOR(S): Clive, Derrick L. J.; Tao, Yong; Khodabocus, Ahmad; Wu, Yong Jin; Angoh, A. Gaetan; Bennett, Sharon M.; Boddy, Christopher N.; Bordeleau, Luc; Kellner, Dorit; et al.

CORPORATE SOURCE: Dep. Chem., Univ. Alberta, Edmonton, AB, T6G 2G2, Can.

SOURCE: Journal of the Chemical Society, Chemical

Communications (1992), (20), 1489-90

CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB (+)-Fredericamycin A (I) is synthesized using 5-exo-diagonal radical closure of selenide II and an unusual procedure for both selective demethylation and adjustment of the stereochem. in the pentadienyl side chain of the advanced intermediate III.

IT 145223-00-3P

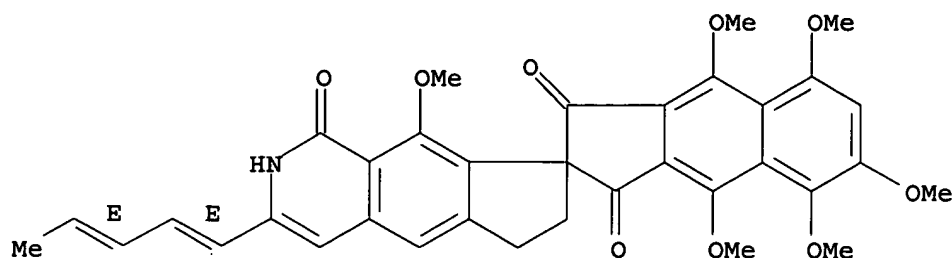
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and deprotection of)

RN 145223-00-3 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 6',7'-dihydro-4,5,6,8,9,9'-hexamethoxy-3'-(1E,3E)-1,3-pentadienyl-(9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1987:49879 CAPLUS
 DOCUMENT NUMBER: 106:49879
 TITLE: Fredericamycin A derivatives
 INVENTOR(S): Hasegawa, Hiroshi; Yokoi, Koichi; Narita, Masa;
 Asaoka, Takemitsu; Kukita, Kenichi; Ishizeki, Seiji;
 Nakajima, Toshiaki
 PATENT ASSIGNEE(S): S. S. Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61044867	A2	19860304	JP 1984-166283	19840808
JP 03004548	B4	19910123		
PRIORITY APPLN. INFO.:			JP 1984-166283	19840808
OTHER SOURCE(S):	CASREACT 106:49879			
GI				

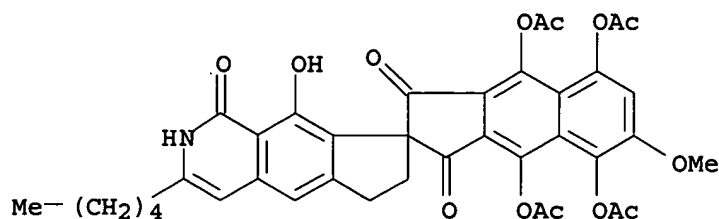
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Stable fredericamycin A derivs. I (R = H, C1-4 alkyl; R1 = C1-4 alkyl), useful as neoplasm inhibitors, were prepared Thus, fredericyamin A (II) was reduced over 10% Pd/C in THF at room temperature for 10 h, then stirred with Ac2O for 1 h to give 80% III. III was heated with MeI and Ag2O in Me2CO for 1 h to give 56.3% I (R = R1 = Me), whose i.p. administration prolonged the lives of mice transplanted with Ehrlich cancer cells (5 + 10⁶ cells/animal) in a dose dependent manner. A saline solution of III was more stable than that of II.

IT 97854-12-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and alkylation of)

RN 97854-12-1 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 4,5,8,9-tetrakis(acetyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-pentyl- (9CI) (CA INDEX NAME)



L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1986:33948 CAPLUS
 DOCUMENT NUMBER: 104:33948
 TITLE: Fredericamycin A derivatives
 INVENTOR(S): Yokoi, Koichi; Hasegawa, Hiroshi; Narita, Masa;
 Asaoka, Takemitsu; Kukita, Kenichi; Ishizeki, Seiji;
 Nakajima, Toshiaki
 PATENT ASSIGNEE(S): S. S. Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 60152468	A2	19850810	JP 1984-6746	19840118
PRIORITY APPLN. INFO.:			JP 1984-6746	19840118

OTHER SOURCE(S): CASREACT 104:33948

GI For diagram(s), see printed CA Issue.

AB Title compds. I (R = acyl, X = Q, Q1), useful as neoplasm inhibitors (no data), were prepared. Thus, fredericamycin A was reduced with H2 in THF in the presence of 10% Pd/C to give 60% tetrahydrofredericamycin A, which was treated with n-lauric anhydride in pyridine to give 75.6% I (R = n-lauroyl, X = Q).

IT 97854-13-2P 97854-14-3P 97867-37-3P
 97867-38-4P

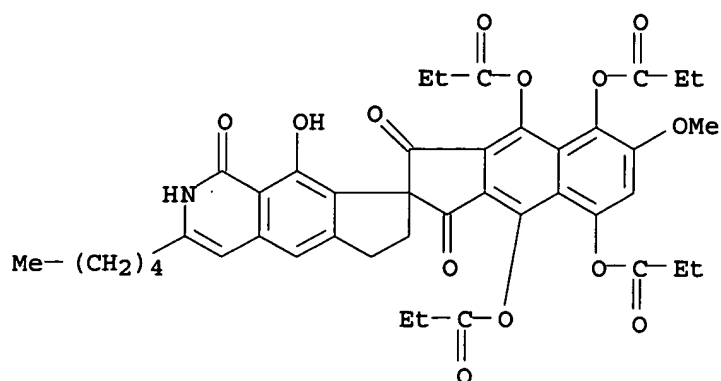
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of, as neoplasm inhibitor)

RN 97854-13-2 CAPLUS

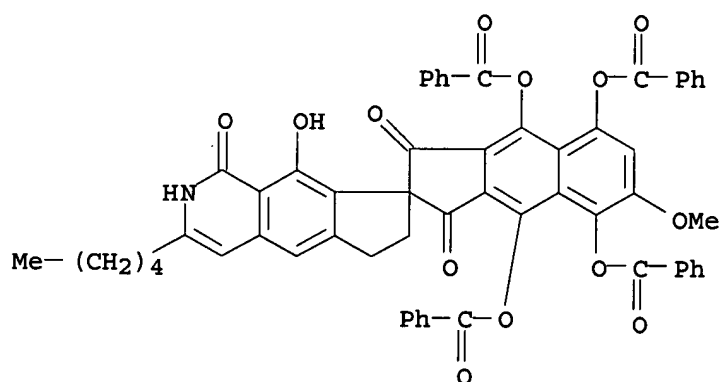
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 6',7'-dihydro-9'-hydroxy-6-methoxy-4,5,8,9-tetrakis(1-oxopropoxy)-3'-pentyl- (9CI) (CA INDEX NAME)

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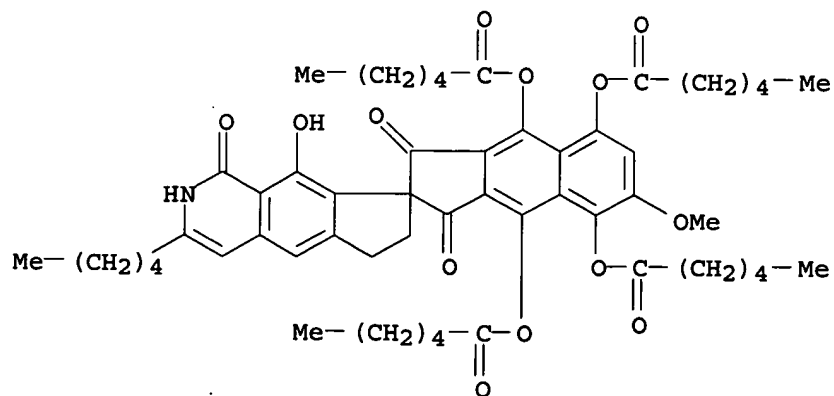
RN 97854-14-3 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-trione, 4,5,8,9-tetrakis(benzoyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-pentyl- (9CI) (CA INDEX NAME)



RN 97867-37-3 CAPLUS

CN Hexanoic acid, 1,1',2',3,6',7'-hexahydro-9'-hydroxy-6-methoxy-1,1',3-trioxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,5,8,9-tetrayl ester (9CI) (CA INDEX NAME)



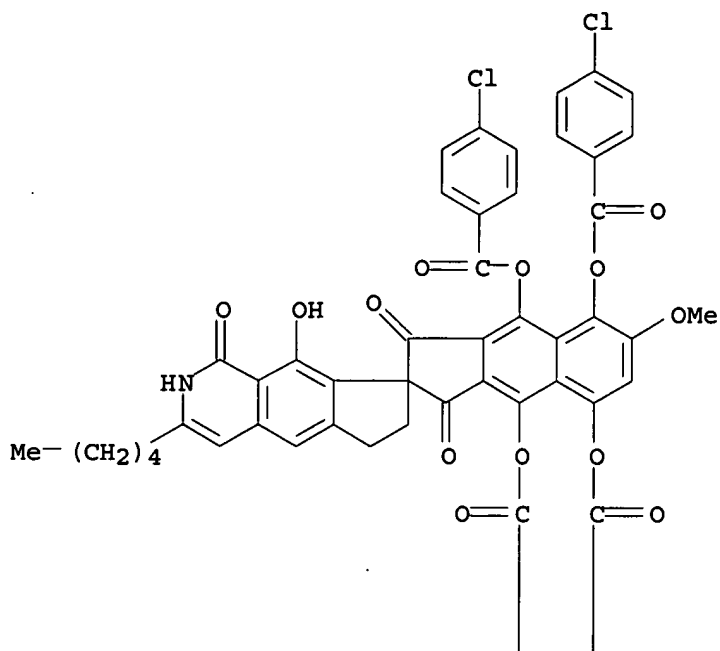
RN 97867-38-4 CAPLUS

CN Benzoic acid, 4-chloro-, 1,1',2',3,6',7'-hexahydro-9'-hydroxy-6-methoxy-

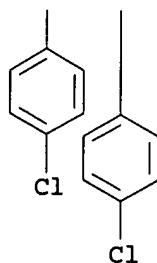
10/520,421

1,1',3-trioxo-3'-pentylspiro[2H-benz[f]indene-2,8'-
[8H]cyclopent[g]isoquinoline]-4,5,8,9-tetrayl ester (9CI) (CA INDEX NAME)

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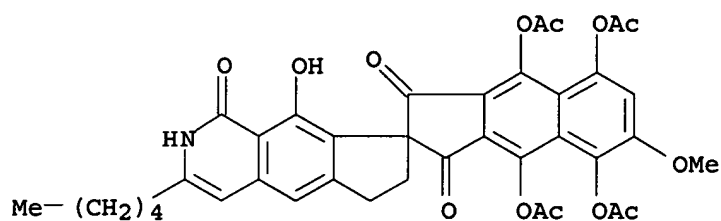
PAGE 2-A



L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:504798 CAPLUS
DOCUMENT NUMBER: 103:104798
TITLE: Fredericamycin A derivative
INVENTOR(S): Yokoi, Koichi; Hasegawa, Hiroshi; Narita, Tadashi;
Asaoka, Takemitsu; Kurita, Kenichi; Ishizeki, Seiji;
Nakashima, Toshiaki
PATENT ASSIGNEE(S): S. S. Pharmaceutical Co., Ltd., Japan
SOURCE: Ger. Offen., 44 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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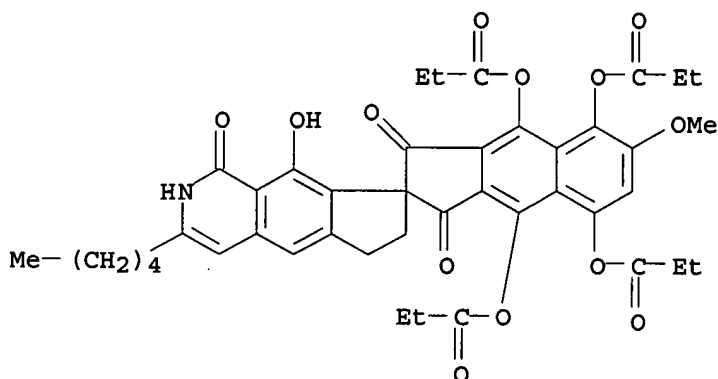
IT 97854-13-2P 97854-14-3P 97867-37-3P

97867-38-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

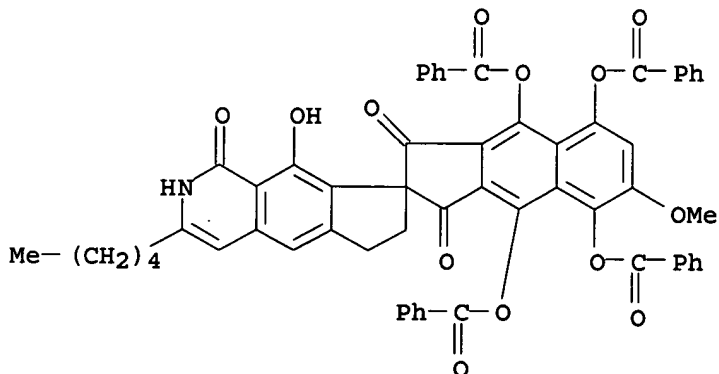
RN 97854-13-2 CAPLUS

CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-
trione, 6',7'-dihydro-9'-hydroxy-6-methoxy-4,5,8,9-tetrakis(1-oxopropoxy)-
3'-pentyl- (9CI) (CA INDEX NAME)



RN 97854-14-3 CAPLUS

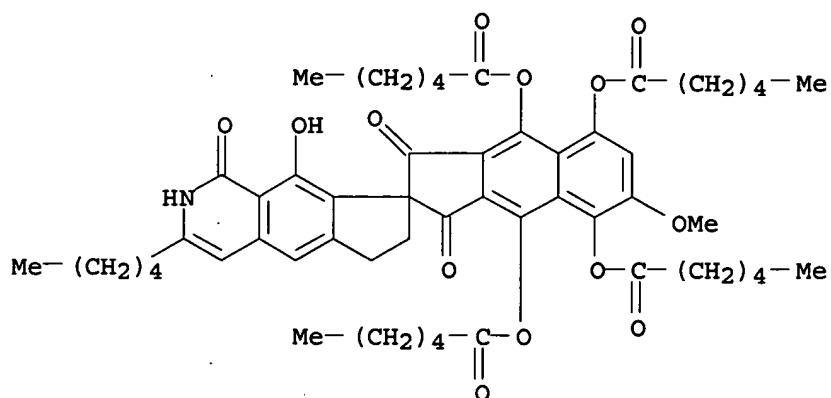
CN Spiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-1,1',3(2'H)-
trione, 4,5,8,9-tetrakis(benzoyloxy)-6',7'-dihydro-9'-hydroxy-6-methoxy-3'-
pentyl- (9CI) (CA INDEX NAME)



RN 97867-37-3 CAPLUS

CN Hexanoic acid, 1,1',2',3,6',7'-hexahydro-9'-hydroxy-6-methoxy-1,1',3-
trioxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-
4,5,8,9-tetrayl ester (9CI) (CA INDEX NAME)

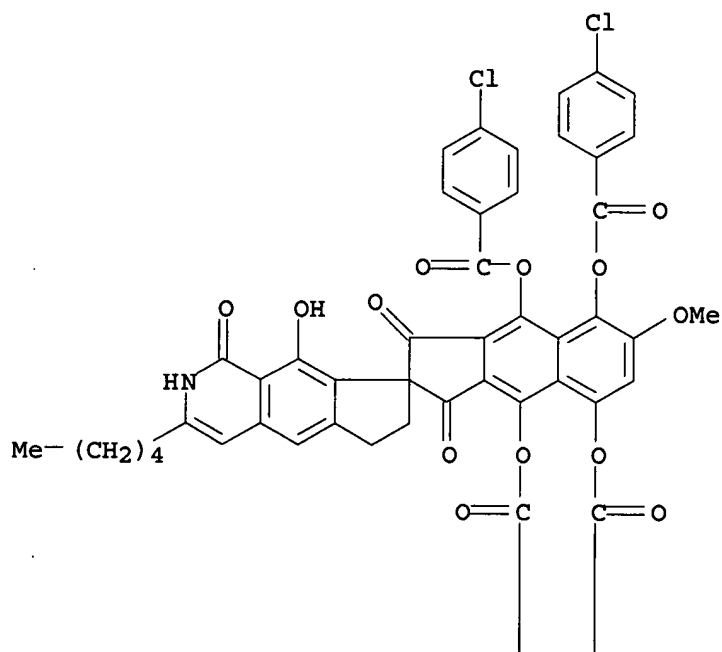
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RN 97867-38-4 CAPLUS

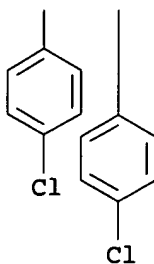
CN Benzoic acid, 4-chloro-, 1,1',2',3,6',7'-hexahydro-9'-hydroxy-6-methoxy-1,1',3-trioxo-3'-pentylspiro[2H-benz[f]indene-2,8'-[8H]cyclopent[g]isoquinoline]-4,5,8,9-tetrayl ester (9CI) (CA INDEX NAME)

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PAGE 2-A



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FILE 'REGISTRY' ENTERED AT 10:40:10 ON 16 AUG 2006

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 0 S L1 FULL

L4 STRUCTURE UPLOADED

L5 0 S L4

L6 13 S L4 FULL

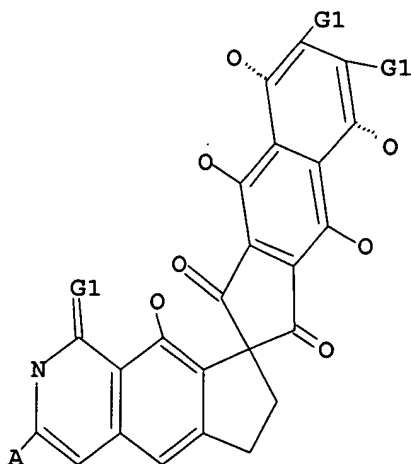
FILE 'CAPLUS' ENTERED AT 10:42:10 ON 16 AUG 2006

L7 9 S L6

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L1 HAS NO ANSWERS

L1 STR



G1 O,S,N

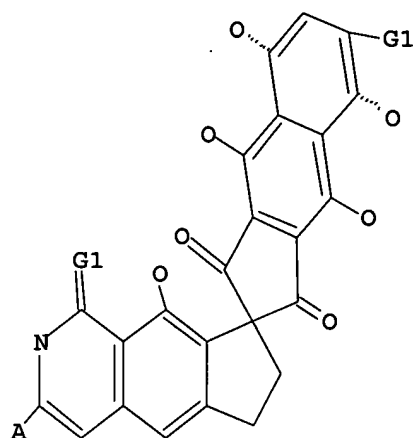
Structure attributes must be viewed using STN Express query preparation.

=> d l4

L4 HAS NO ANSWERS

L4 STR

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G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> => d his

(FILE 'HOME' ENTERED AT 10:39:52 ON 16 AUG 2006)

FILE 'REGISTRY' ENTERED AT 10:40:10 ON 16 AUG 2006

L1	STRUCTURE UPLOADED
L2	0 S L1
L3	0 S L1 FULL
L4	STRUCTURE UPLOADED
L5	0 S L4
L6	13 S L4 FULL

FILE 'CAPLUS' ENTERED AT 10:42:10 ON 16 AUG 2006

L7	9 S L6
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FILE 'REGISTRY' ENTERED AT 10:43:12 ON 16 AUG 2006

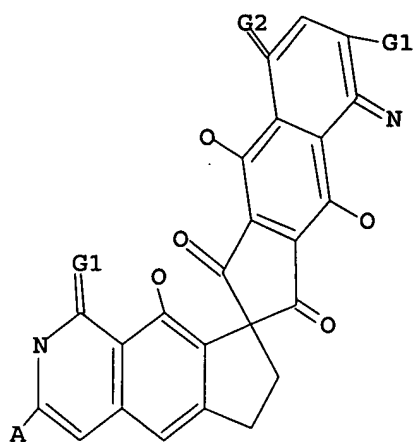
L8	STRUCTURE UPLOADED
L9	0 S L8
L10	STRUCTURE UPLOADED
L11	0 S L10

=> d 18

L8 HAS NO ANSWERS

L8	STR
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G1 O,S,N

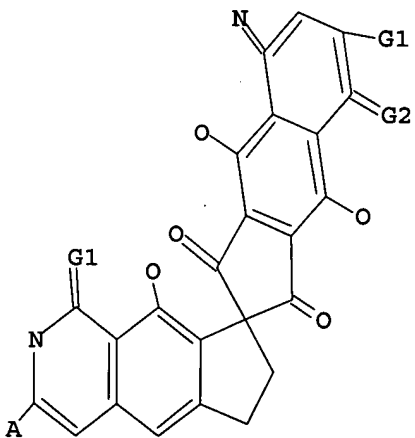
G2 O,N

Structure attributes must be viewed using STN Express query preparation.

=> d l10

L10 HAS NO ANSWERS

L10 STR



G1 O,S,N

G2 O,N

Structure attributes must be viewed using STN Express query preparation.

=>